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# EXTENDED X-RAY ABSORPTION FINE STRUCTURE STUDY OF BOND CONSTRAINTS IN GE-SB-TE ALLOYS

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In work performed by researchers in the Physics Department at NC State University, studies of the local structure of GeSbTe alloys were studied using Extended X-Ray Absorption Spectroscopy, or EXAFS. Using the spectroscopic capabilities provided by the MCAT line at the Advanced Photon Source at Argonne National Laboratory, examination of the absorption edges of all three elements Ge, Sb and Te were investigated. This effort was de-scoped because AFOSR dropped funding after one year.

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In work performed by researchers in the Physics Department at NC State University, studies of the local structure of GeSbTe alloys were studied using Extended X-Ray Absorption Spectroscopy, or EXAFS. Using the spectroscopic capabilities provided by the MCAT line at the Advanced Photon Source at Argonne National Laboratory, examination of the absorption edges of all three elements Ge, Sb and Te were investigated.

In these studies, principal results involved determination and interpretation of the nearest neighbor numbers $N$ and bond distances $r$ for each species. Results were internally consistent in that the Te nearest neighbor distances NTe-Sb = 2.83Å and NTe-Ge = 2.62Å were the same whether measured from the Te atom or the neighboring (Ge or Sb) atom. Co-ordination numbers $N$ likewise agree for all species measured. The proximity of the Sb and Te edges (atomic numbers 51 and 52 respectively) makes it difficult to distinguish Te-Te and Te-Sb bonds, nonetheless several clear distinctions can be made.

In Ge2Sb2Te5 results suggest that the fundamental local units are Ge2Te3, Ge17Te83 and Sb2Te3 with essentially all Ge bonded in Ge2Te3 structures. The Ge17Te83 structures were found to possess considerable Te-Te bonding. Using Bond Constraint Theory, BCT, these data on local bonding configurations allow one to calculate the average number of constraints per atom in Ge2Sb2Te5. In particular the presence of Ge-Ge bonds and the fact that Te bending constraints can be removed indicate an average number of constraints per atom of 2.38 which is close to the ideal number of 2.4 as per the theory of J.C. Phillips and P. Boulchand. At this value, it is argued that one has an ideal balance between local stress without the percolation of stress through the solid matrix.

BCT argues that low coordination results in a floppy material that would allow for easy glass formation but the steric freedom of such a solid would allow for a plethora of defect states. As coordination is increased bond constraint increases and pockets of rigidity begin to grow. When these pockets of rigidity percolate the material become stressed rigid. It is argued that a narrow range of materials between these extremes exists in a so-called intermediate phase of ideal constraints. Material in this regime should be good glass formers and may exhibit reversible photo- or electrically- induced transitions between amorphous and crystalline phases.

Possessed as it is of an ideal number of constraints, Ge2Sb2Te5 is a good glass-former with an ability to make rapid and reversible transitions between the amorphous and crystalline phases. The ideal nature of Ge2Sb2Te5 can also be argued by appealing to this material's position on the Ge-Sb-Te ternary composition diagram. On this diagram, Ge2Sb2Te5 can be argued to be a pseudo-binary because it lies at the intersection of two tie-lines: one connecting GeTe and Sb2Te3 and another connecting Te with GeSb.

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